N-Nitrosodiethylamine, HFBA-derivative

Inchi: InChI=1S/C12H6F14N2O2/c1-3-27(4-2)28(5(29)7(13,14)9(17,18)11(21,22)23)6(30)8(15,
InchiKey: PFBZCIAYISYXMP-UHFFFAOYSA-N
Formula: C12H6F14N2O2
SMILES: C=CN(C=C)N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 476.17

Physical Properties

Property code	Value	Unit	Source
gf	-2520.74	kJ/mol	Joback Method
hf	-2928.29	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	39.33	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.511		Crippen Method
mcvol	219.220	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
tb	570.34	K	Joback Method
tc	712.71	K	Joback Method
tf	409.06	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.80	J/mol×K	570.34	Joback Method
cpg	638.41	J/mol×K	594.07	Joback Method
cpg	649.09	J/mol×K	617.80	Joback Method
cpg	658.91	J/mol×K	641.52	Joback Method
cpg	667.93	J/mol×K	665.25	Joback Method
cpg	676.20	J/mol×K	688.98	Joback Method
cpg	683.80	J/mol×K	712.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R579918&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume